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Integral approximants

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Abstract

The approximation problem for multivalued functions on the complex plane is discussed. A sub-class of Hermite–Padé approximants is defined and the supporting theory is developed, inspired by the Riemann monodromy theorem. It is plausibly shown that the method can resolve confluent singularities. The application of the method tested on realistic series gives promises for the method.

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Keywords: Monodromy; Riemann's theorem; Hermite–Padé approximants; Riemann sheet; Series expansions; Confluent singularity

PROGRAM SUMMARY

Title of program: IA

Catalogue identifier: ADEH

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Licensing provisions: none

Computers: DEC MicroVAX 3300, or DEC 3000 ALPHA 300 AXP

Operating systems under which the program has been tested: VAX/VMS V5.5, or DEC OSF/1 AXP

Programming language used: FORTRAN 77

No. of bytes in distributed program, including test data, etc.: 191082

Distribution format: ASCII

Keywords: Monodromy, Riemann's theorem, Hermite–Padé approximants, Riemann sheet, series expansions, confluent singularity

Nature of the physical problem

We present a novel method of approximating multivalued functions on multiple Riemann sheets, defined by a finite number of coefficients in a power series expansion. The method is effective in representing singularities of a complex structure expected in functions anticipated in the study of critical thermodynamic behavior. The FORTRAN program is described in some details.

Method of solution

The method relies on the Riemann's monodromy theorem for monogenic analytic functions.

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LONG WRITE-UP

1. Introduction

The problem of gaining information about the analytic structure of a function, represented by a finite number of coefficients of a power series expansion, is a very common problem in many areas of physics, especially in the theory of critical phenomena. One is usually interested in estimating the location and the nature of the dominant singularities of the function. The method of (ordinary) Padé approximants [1] has offered for the last 30 years exact information, provided that the behavior of the function is sufficiently simple, for example, simple poles or isolated branch points are present. However, more singular behavior, such as the presence of confluent singularities or singularities of the Kosterlitz–Thouless type, cannot be represented exactly in terms of the Padé method. These problems have led to the development of more sophisticated methods of series analysis, as the integral approximants methods, which belong to the general family of the Hermite–Padé approximants (HPA) [2,3]. The method is based on the construction of an inhomogeneous linear differential equation with polynomial coefficients determined from the series expansion of the function and the approximants are the solutions of the equation. Specifically, we try to implement here in a formal fashion the ideas of monodromy and Riemann's theorem from the classical analysis of functions of a complex variable into the Hermite–Padé approximation theory.

To make that idea more clear, suppose that we are given the first $(N + 1)$ coefficients of the power series expansion,

$$f(z) = \sum_{n=0}^{\infty} a_n z^n. \quad (1.1)$$

We can construct the polynomials $P(z)$, $Q(z)$, \dots , $S(z)$, $T(z)$ of degrees p, q, \dots, s, t , respectively, such that the equation

$$P(z) \frac{d^m f}{dz^m} + Q(z) \frac{d^{m-1} f}{dz^{m-1}} + \dots + S(z) f + T(z) = 0 (z^{N+1}) \quad (1.2)$$

is satisfied to order N , where $m + p + q + \dots + s + t = N + 1$, with the normalization condition $P(0) = 1$. We then define as *integral approximants*, denoted by

$$y(z) \equiv [t/s, \dots, q, p], \quad (1.3)$$

the solution of the differential equation

$$P(z) \frac{d^m f}{dz^m} + Q(z) \frac{d^{m-1} f}{dz^{m-1}} + \dots + S(z) f + T(z) = 0, \quad (1.4)$$

with the initial conditions $y(0) = f(0)$, $y'(0) = f'(0)$, \dots , $y^{(m-1)}(0) = f^{(m-1)}(0)$. The polynomials P, Q, \dots, S, T are called *Hermite–Padé polynomials*. The singularity structure of the function $y(z)$ will then provide the estimates of the singularity structure of the unknown function $f(z)$.

Section 2 is devoted to a brief review of the classical theory of multivalued functions of a complex variable, introduces the idea of monodromy based on the classical theory of functions by Riemann and relates this idea to the analysis of series. Section 3 gives the formulae that are used to derive the numerical approximation theory in the series analysis problem. Section 4 contains a general description of the program and assembles various remaining details of the algorithm. Test runs for various test functions and applications to realistic problems appear in Section 5 to demonstrate the validity of the method and finally in Section 6 a summary of general remarks concludes the paper.

2. Classical Riemann problem and the monodromy group

We will review in this section some aspects of the classical theory of functions of a complex variable [4]. Suppose we have a formal power series about z_0 ,

$$f(z, z_0) = \sum_{n=0}^{\infty} a_n (z - z_0)^n, \quad (2.1)$$

convergent in a disk on nonzero radius of convergence. By standard analytic continuation, we can construct the m linearly independent coverings of the complex plane, y_1, y_2, \dots, y_m , which are regular in the neighborhood of z_0 , where m depends on (2.1) and the truth of this statement depends on the absence of a natural barrier. The pairs

$$(z_0, w_0^{(1)}), (z_0, w_0^{(2)}), \dots \quad (2.2)$$

constitute the monogenic analytic function generated by the original series representation of the function, where $w_0^{(n)} = y_n(z_0, z_0)$. The number of independent coverings m is finite or at most denumerably infinite and it is called the *monodromic dimension* of the monogenic analytic function.

Suppose a monogenic function of monodromic dimension m has exactly n singular points in the extended complex plane, a_1, a_2, \dots, a_n , including also the point at infinity. If z_0 is a regular point, we can construct by analytic continuation the m linearly independent coverings of the complex plane, y_1, y_2, \dots, y_m , in the neighborhood of z_0 . By encircling in the positive direction the i th singular point a_i , the system of coverings $y = (y_1, y_2, \dots, y_m)$ is transformed into a new set of functions $Y = (Y_1, Y_2, \dots, Y_m)$, where

$$Y_j(z) = \sum_{k=1}^m M_{jk}^{(i)} y_k(z), \quad (2.3)$$

since the transformation $y \rightarrow Y$ represents an analytic continuation of the original function and any such a transformation must be a linear combination of the basis functions $y = (y_1, y_2, \dots, y_m)$. The $m \times m$ matrix $M^{(i)}$ is called a *monodromy matrix* and by an application of Cauchy's theorem, one can prove that

$$M^{(1)} M^{(2)} \dots M^{(n)} = I. \quad (2.4)$$

From this relation it follows that for every matrix $M^{(i)}$ there is an inverse, representing a circulation in the negative direction. It is obvious that circulation on the complex plain around a circle not enclosing any singular points does not change the function. Therefore, these matrices generate a group \mathcal{M} , called the *monodromy group* of the system $y = (y_1, y_2, \dots, y_m)$.

A simple example can be given to illustrate these ideas. Take the function

$$f(x) = (1-x)^{-3/2} + (1+x)^{-5/4},$$

which has three singular points at $z = \pm 1, \infty$. If we encircle once the singular point $z = 1$ in the positive direction, we generate a new function

$$f_1(x) = (1-x)^{-3/2} e^{2\pi i 3/2} + (1+x)^{-5/4} = -(1-x)^{-3/2} + (1+x)^{-5/4}$$

and encircling the singularity $z = 1$ once more, we obtain

$$f_2(x) = (1-x)^{-3/2} + (1+x)^{-5/4} = f(x).$$

Repeating this procedure for $x = -1$ or ∞ , we always end up with the functions f_1 or f_2 . We can then choose these two functions as the basis functions for spanning the Riemann surface. Encircling any of the three

singular points, the basis functions (f_1, f_2) are transformed according to Eq. (2.3) and it is easy to calculate the following monodromy matrices:

$$M^{(+1)} = \begin{pmatrix} 0, & 1 \\ 1, & 0 \end{pmatrix}, \quad M^{(-1)} = \begin{pmatrix} 1-i, & -1-i \\ -1-i, & 1-i \end{pmatrix}, \quad M^{(\infty)} = \begin{pmatrix} -1+i, & 1+i \\ 1+i, & -1+i \end{pmatrix}.$$

The problems we are dealing with here have roots in the *Riemann–Hilbert monodromy problem*. Riemann formulated this problem as follows [5]: *Given a set of singular points $\{a_1, a_2, \dots, a_n\}$ and a set of matrices $\{M^{(1)}, M^{(2)}, \dots, M^{(n)}\}$, find a system of functions $y = (y_1, y_2, \dots, y_m)$, such that (i) y has singularities only at the points $\{a_1, a_2, \dots, a_n\}$ and (ii) the monodromy group of y coincides with the monodromy group generated by the matrices $\{M^{(1)}, M^{(2)}, \dots, M^{(n)}\}$.* In 1857 Riemann solved this problem (even though he overlooked at the existence of a solution for the problem) and later in 1912 Hilbert [6] gave the first serious solution for the $m = 2$ case. Since then, many other scientists have given solutions with different approaches.

In Riemann's notations, any system of functions that satisfies these arguments belongs to a class of functions, denoted by

$$\mathcal{Q} \left(\begin{matrix} a_1, a_2, \dots, a_n \\ M^{(1)}, M^{(2)}, \dots, M^{(n)}; z \end{matrix} \right). \quad (2.5)$$

In addition, Riemann assumed that the functions y have *singularities of finite order*, which means that every function y_j behaves at the singular point a_i as follows:

$$\left| \frac{y_j'}{y_j} \right| \leq \frac{A}{|z - a_i|^r} \quad (2.6)$$

for finite r and A . We can state now the *Riemann's monodromy theorem*:

For each $m+1$ systems of functions y_j ; $j = 1, 2, \dots, m+1$ belonging to the same class \mathcal{Q} , there exists a linear homogeneous relation with polynomial coefficients, such that

$$\sum_{j=1}^{m+1} A_j(z) y_j(z) = 0. \quad (2.7)$$

As a corollary it follows that if y is an element of the class \mathcal{Q} , then so also are $y', y'', \dots, y^{(m)}$, as can be seen by differentiating the monodromy group equations (2.3). Therefore, Eq. (2.7) is written for the system

$$A_0 + A_1 y_k^{(1)} + \dots + A_m y_k^{(m)} = 0, \quad k = 1, 2, \dots, m. \quad (2.8)$$

In other words, we produce Eq. (1.4). We conclude that for functions from the class \mathcal{Q} , the integral approximants yield exact results, providing the approximation procedure is carried out to the adequate order of the polynomials $\{A_i\}$. Therefore, it seems reasonable to study the approximation scheme in the context of monodromy. Actually it can be shown that the integral approximants cannot converge on more Riemann sheets simultaneously than can be accommodated by the monodromic dimension of the solution of the differential equation defining the approximant.

Very often we lack the global information about a function $f(z)$. In that case we can define the local monodromic dimension (and state an analogous Riemann theorem) as follows: given a convergent series expansion about a point $z = z_0 = 0$ in the disk of convergence $\mathcal{D} = \{z; |z| \leq R\}$, we say that $f(z)$ has *local monodromic dimension m* , if the analytic continuation along any path in \mathcal{D} generates exactly m linearly independent coverings in \mathcal{D} .

3. Computational method

3.1. Confluent singularity case

We will illustrate next the application of the proposed method to the problem of confluent singularities using a 2nd order inhomogeneous differential equation,

$$P(z) \frac{d^2 y}{dz^2} + Q(z) \frac{dy}{dz} + R(z)y + U(z) = 0. \quad (3.1)$$

In the theory of critical phenomena, many thermodynamic quantities behave in the vicinity of the critical points z_c as follows:

$$f(z) = \phi_1(z)|z - z_c|^{\gamma_1} + \phi_2(z)|z - z_c|^{\gamma_2} + \phi_0(z), \quad (3.2)$$

where $0 < \gamma_2 < \gamma_1$, $\gamma_1 - \gamma_2 \neq \text{integer}$, and $\phi_i(z_c) \neq 0, \infty$. Since there are three independent coverings in (3.2), counting also the analytic background term, it might seem more appropriate to work with a 3rd order homogeneous differential equation instead, but the solution of (3.1) includes the form (3.2). From the standard theory of differential equations we expect for this case the polynomial $P(z) \propto (z - z_c)^2$. In practice usually we get two single zeros of $P(z)$ clustered around z_c instead of a double zero at $z = z_c$. We reason that as the approximation picture improves, these zeros should merge into z_c . There remains always the problem of distinguishing between a true confluent singularity and two or more nearby separate singularities.

As an example, the following function displays a confluence at $z = 1$:

$$f(z) = (1 - z)^{-7/4} + (1 - z)^{-5/4} + e^{-z}$$

and has a local monodromic dimension $m = 2$ plus an analytic background in a disk of convergence $|z| \leq 2$ (the global monodromic dimension is 3). It is elementary to show this function satisfies the 2nd order differential equation,

$$(1 - z)^2 y'' - 4(1 - z)y' + \frac{35}{16}y = (z^2 - 6z + \frac{115}{16})e^{-z}.$$

From the zeros of $P(z)$, we select a pair of nearby zeros, z_1, z_2 (complex or real), and by transforming Eq. (3.1) into a system of 1st order ODE's, we integrate the system starting out from the origin, with initial conditions $y(0) = f(0)$ and $y'(0) = f'(0)$, up to a point z close to the nearest singularity to the origin, thus obtaining $y(z)$. We next integrate counterclockwise $(2m + 1)$ times around a close contour that encloses both singularities (and no others). This procedure will generate the coverings $y_1(z), y_2(z), y_3(z), y_4(z), y_5(z)$, interrelated by Eq. (2.3),

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} = \mathcal{M} \begin{pmatrix} y \\ y_1 \\ y_2 \end{pmatrix}, \quad \begin{pmatrix} y_2 \\ y_3 \\ y_4 \end{pmatrix} = \mathcal{M} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}, \quad \begin{pmatrix} y_3 \\ y_4 \\ y_5 \end{pmatrix} = \mathcal{M} \begin{pmatrix} y_2 \\ y_3 \\ y_4 \end{pmatrix}, \quad (3.3)$$

whence we produce the 3×3 monodromy matrix \mathcal{M} . Diagonalizing this matrix we get

$$U\mathcal{M}U^{-1} = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad (3.4)$$

where the unity eigenvalue corresponds to the analytic background in (3.2). From these eigenvalues we can calculate the confluence exponents of (3.2),

$$\gamma_j = \frac{\ln \lambda_j}{2\pi i}, \quad j = 1, 2. \quad (3.5)$$

A problem arises at this point, since this equation does not define which Riemann sheet of the logarithmic function has to be chosen. To resolve this problem, we can use an approximate method to calculate the exponent γ_j . If we take a Taylor expansion of the polynomials $P(z)$, $Q(z)$, $R(z)$ in (3.1) about the singular points z_1 and z_2 and we look for solutions in the form $\phi(z)(z - z_c)^\beta$, we calculate the *local singularity indices*

$$\beta_1 = 1 - \frac{Q(z_1)}{P'(z_1)}, \quad \beta_2 = 1 - \frac{Q(z_2)}{P'(z_2)}, \quad (3.6)$$

and the auxiliary indices

$$s_1 = \frac{R(z_1)}{\lim_{z \rightarrow z_1} P(z)/(z - z_1)(z - z_2)}, \quad s_2 = \frac{R(z_2)}{\lim_{z \rightarrow z_2} P(z)/(z - z_1)(z - z_2)}. \quad (3.7)$$

From these we get the *approximate critical exponents*

$$\gamma_j = -\frac{1}{2}[(\beta - 1) \pm \sqrt{(\beta - 1)^2 - 4s}], \quad j = 1, 2, \quad (3.8)$$

where

$$\beta = 2 - \beta_1 - \beta_2, \quad s = \frac{1}{2}(s_1 + s_2). \quad (3.9)$$

These values should suffice to determine the correct Riemann sheet.

The amplitudes in (3.2), $\phi_0(z)$, $\phi_1(z)$, $\phi_2(z)$, can be calculated by integrating around the pair z_1, z_2 as described previously. Rehr et al. [7] suggested that the difference $z_1 - z_2$ is a measure of the error in estimating z_c . Let us write the solution $y(z)$ in a separated form in analogy to (3.2),

$$y(z) = y_+(z) + y_-(z) + y_0(z). \quad (3.10)$$

This decomposition can be computed in terms of the coverings $y(z)$, $y_1(z)$, $y_2(z)$ and the eigenvalues of the monodromy matrix \mathcal{M} . Thus, circulating around the pair of zeros (z_1, z_2) n times we reproduce the coverings

$$y_n(z) = y_+(z)\lambda_1^n + y_-(z)\lambda_2^n + y_0(z), \quad (3.11)$$

where the eigenvalues λ_1, λ_2 have been calculated previously. Hence we get

$$\begin{aligned} y_+(z) &= \frac{\lambda_2(y - y_1) - (y_1 - y_2)}{(\lambda_2 - \lambda_1)(1 - \lambda_1)}, \\ y_-(z) &= \frac{\lambda_1(y - y_1) - (y_1 - y_2)}{(\lambda_1 - \lambda_2)(1 - \lambda_2)}, \\ y_0(z) &= y(z) - y_+(z) - y_-(z). \end{aligned} \quad (3.12)$$

Asymptotically as $z \rightarrow z_c$, we expect a behavior (at distances $r \ll 1$, but $r \gg |z_1 - z_2|$) of the form

$$\begin{aligned} y_+(z) &\approx \phi_1(z)(z - z_c)^{\gamma_1}, \\ y_-(z) &\approx \phi_2(z)(z - z_c)^{\gamma_2}, \\ y_0(z) &\approx \phi_0(z), \end{aligned} \quad (3.13)$$

where ϕ_j are analytic functions at z_c . To obtain the amplitudes and the residues of (3.2), we calculate by integration of (3.1) the quantities

$$\begin{aligned} \phi_1(z) &= y_+(z)(z - z_c)^{-\gamma_1}, \\ \phi_2(z) &= y_-(z)(z - z_c)^{-\gamma_2}, \\ \phi_0(z) &= y_0(z), \end{aligned} \quad (3.14)$$

and extrapolating these functions to the point z_c as follows:

$$\phi_j(z_c) \approx \phi_j(z) + \phi'_j(z)(z_c - z) + 0((z_c - z)^2), \quad j = 0, 1, 2, \quad (3.15)$$

we obtain

$$\phi_j(z_c) \approx (1 - \lambda_j)y_{\pm}(z)(z - z_c)^{-\gamma_j} - y'_{\pm}(z)(z - z_c)^{1-\gamma_j}, \quad j = 1, 2, \quad (3.16)$$

where the derivatives $y'_{\pm}(z)$ and $\phi'_0(z)$ are calculated by the integration of (3.1).

3.2. Isolated nonconfluent singularity case

In the case of a single isolated singularity at z_c , we expect $P(z_c) = 0$ and $P'(z_c) \neq 0$ in (3.1). The function in the vicinity of the singularity has the structure

$$f(z_c) = \phi_1(z)(z - z_c)^{\beta} + \phi_0(z), \quad (3.17)$$

where $\phi_j(z)$ is analytic at z_c and the singularity exponent β is given by (3.6), i.e.,

$$\beta = 1 - \frac{Q(z_c)}{P'(z_c)}. \quad (3.18)$$

In order to calculate the amplitude and the residue in (3.17) at $z = z_c$, we expand the polynomials in (3.1), $P(z)$, $Q(z)$, $R(z)$, $U(z)$, in powers about $\xi = 0$ where $\xi = z - z_c$ and we calculate the coefficients of the following series solutions by fitting in the homogeneous version of (3.1) for $\beta \neq 0$ and $\beta = 0$, respectively:

$$\begin{aligned} y_{\beta}(\xi) &= \xi^{\beta} \sum_{n=0}^{\infty} a_n \xi^n, \\ y_0(\xi) &= \sum_{n=0}^{\infty} b_n \xi^n, \end{aligned} \quad (3.19)$$

with the conditions $a_0 = b_0 = 1$ and similarly from the inhomogeneous equation (3.1) we calculate

$$y_{00}(\xi) = \sum_{n=0}^{\infty} c_n \xi^n, \quad (3.20)$$

with the condition $y_{00}(0) = c_0 = 0$. Next we integrate (3.1) from the origin to some intermediate point z close to z_c ($|z| < |z_c|$), where we expect Eqs. (3.19), (3.20) to converge rapidly, thus producing $y(z)$ and $y'(z)$. Since the expected behavior of $y(z)$ is of the form

$$\begin{aligned} y(z) &= A_{\beta} y_{\beta}(\xi) + A_0 y_0(\xi) + y_{00}(\xi), \\ y'(z) &= A_{\beta} y'_{\beta}(\xi) + A_0 y'_0(\xi) + y'_{00}(\xi). \end{aligned} \quad (3.21)$$

these equations can be solved with respect to A_{β} and A_0 ,

$$\begin{aligned} A_{\beta} &= \frac{y'_0(y - y_{00}) - y_0(y' - y'_{00})}{y_{\beta} y'_0 - y'_{\beta} y_0}, \\ A_0 &= -\frac{y'_{\beta}(y - y_{00}) - y_{\beta}(y' - y'_{00})}{y_{\beta} y'_0 - y'_{\beta} y_0}, \end{aligned} \quad (3.22)$$

where we have dropped the arguments in the rhs of (3.22), i.e., we mean by $y = y(z)$, $y_\beta = y_\beta(\xi)$, etc., and all these quantities have been calculated previously, either by integration or by fitting. From (3.22) it follows immediately the amplitude $\phi_1(z_c) = A_\beta$ and the residue term of (1.16) at $z = z_c$, $\phi_0(z_c) = y_{00}(0) + A_0 = A_0$.

4. The program

The original program was written in FORTRAN language for a CDC CYBER 172 computer and many modifications have been made since then to accommodate newer operating systems supporting standard FORTRAN 77 compilers. The flow of the program is rather simple. The first terms of a series expansion are read and various tasks of series analysis are followed. Running comments have been included in the code to indicate what computation is being done. The program is organized in subroutines, each performing a specific task. There is a header for each subroutine, describing the purpose of its use.

4.1. Input units

The main program IA reads in the first N coefficients of supplied series from logical unit 1, called “HPA.DAT1”,

```
SER(i); i=1,N.
```

The first record in the file contains headings, informative about the series. The various tasks to be performed in the run are contained in logical unit 2, called “HPA.DAT2”. For each task, a dummy variable ADUM and an integer pointer K1 are read in statement number 100,

```
100 READ(2) ADUM,K1.
```

After the assigned task has been executed, control is transferred back to statement 100. The variable ADUM takes on an optional value from the menu below:

```
ADUM='TEST'   Derive test series.
ADUM='READ'   Read in series coefficients from unit 1.
ADUM='TABL'   Form a table of IA approximants of the K1 sequence (cf. [3]).
ADUM='HPA'    Calculate the Hermite-Padé polynomials (P,Q,R,U) of given degrees (LPJ,MPJ,LAJ,
               JPJ) and calculate the physical singularities and the associated indices.
ADUM='RDXC'   Read in K1 probe values for the physical singularities from unit 2. Amplitude calculations
               will be attempted only for those singularities found close to the probes.
ADUM='END'    End current job.
```

The program tape contains at the end the files HPA.DAT1, HPA.DAT2 and TEST.RUN for the test run.

4.2. Output units

As the run proceeds, the program prints out on the logical unit 6, called “HPA.OUT”, the supplied series, the table of approximants to be calculated and for each approximant the HPA polynomials, the singular points and the associated amplitudes and critical indices. During the execution some warning or advisory messages, or accuracy criteria might be printed out. The program tape includes at the end the files HPA.OUT1 and HPA.OUT2, which contain the test run outputs.

4.3. Labelled common blocks

To keep calls to subroutines as uncluttered as possible, variables that remain constant during the calculation of a specific approximant and also calculations related to the same approximant are passed on common blocks,

while variables that change are passed in calls.

The include files, “POLYS.DEG”, “POLYS.ALL”, and “TABLE.IA”, contain common blocks and variable declarations in order to save memory space. If the FORTRAN compiler does not support the INCLUDE statement, one must add to the source program the corresponding common block file, wherever the include statement is called. The include file “POLYS.DEG”,

```
COMMON/BK1/LPJ,MPJ,LAJ,JPJ,MDIM,NFC
```

contains the current degrees (LPJ, MPJ, LAJ, JPJ) of the polynomials (P, Q, R, U), respectively, while the include file “POLYS.ALL”,

```
PARAMETER (MAXDEG=50)
```

```
COMMON/BK2/ P(MAXDEG), Q(MAXDEG), R(MAXDEG), U(MAXDEG)
```

allocates a memory space for saving the current polynomial coefficient.

4.4. Variables

The variable names have been chosen mnemonically thus to reminding one of the variables of Section 3. Most of the calculations are performed in double precision arithmetic, depending on the precision of the library routines and the accuracy of the results sought.

4.4.1. Global variables

We give here a summary of the principle variables which remain unchanged for one run and we specify briefly the purpose of their use:

| | |
|----------|---|
| EPS | Tolerance demanded in the calculations (INPUT). |
| ICONSTRA | A real parameter that monitors the constrained requirement. It takes on the values 1, or 0 (yes/no). |
| IR | Number of roots of the polynomial $P(x)$, i.e. $IR \leq LPJ$. |
| MDIM=2 | Monodromic dimension (INPUT). |
| N1=N+1 | Number of the first coefficients of the series expansion available (INPUT). |
| N2=3 | Dimension of the monodromy matrix. |
| NPADE | Total number of integral approximants. It should hold $NPADE \leq NIA$, where NIA is the dimension of the arrays defined in the include file “TABLE.IA”. |
| NSEQ | Pointer of the sequence of integral approximants to be calculated (INPUT). |
| NZC | Number of probe singular points z_c (INPUT). |

4.4.2. Dummy variables

ADUM, AA(20), THETA, GAMMAJ

4.4.3. Global arrays

| | |
|-----------------------------|---|
| AM(i,j); i,j=1,N2 | Complex monodromy matrix. |
| AMPL0, AMPL1, AMPL2 | Complex critical amplitudes. |
| BETA1(2), BETA2(2), BETA(2) | Complex local critical indices β_1, β_2 , and β . |
| GAMMA1(2), GAMMA2(2) | Complex approximate critical indices γ_1 and γ_2 . |
| GAMMA1(k), GAMMA2(k) | Real vectors storing the critical indices γ_1 and γ_2 , calculated on the k th consecutive Riemann sheet. |
| LAMDA1, LAMDA2 | Eigenvalues λ_1 and λ_2 of the matrix AM. |
| S1(2), S2(2), S(2) | Complex local critical indices s_1, s_2 , and s . |

| | |
|-----------------------------|---|
| $\{WR(i), WI(i)\}; i=1, N2$ | Real vectors representing the real and imaginary part of the eigenvalues of the matrix AM . |
| $\{XR(i), XI(i)\}; i=1, IR$ | Real vectors representing the real and imaginary part of the roots of $P(z)$. |
| $ZCFE(i); i=1, NZC$ | Probe values read in for the singular points (INPUT). |

4.5. Subroutines

Presented here is a menu of routine functions. The high points for some routines carrying out basic tasks are explained. Some of the routines may have been commented out in the code.

| | |
|----------|--|
| APPTAB | Derives a table of integral approximants of the $K1$ sequence. |
| CLEAR | Logical function detecting possible singular points located along the integration path from starting point z_1 to ending point z_2 . |
| COLMAX | Finds the maximum element along the i th column of a 2D array. |
| CONTOUR | Presides over the contour integration along a square closed path. It calls the integration routine CERN routine D208. The latter with minor modifications is included at the end of the code (with the name D208), in case the computer does not support the CERN library. |
| CSYSTEM | Solves a $N \times N$ system of linear equations with complex coefficients. It calls the routine COLMAX2. |
| D208 | (CERN routine MERSON) integrates a system of first order differential equation. |
| DPRQD | Presides over the calculation of the roots of a polynomial. It calls either the IMSL routine ZPOLR, or the CERN routine MULLER for the root computation. Either one of the routines ZPOLR or MULLER can be called for the same purpose. |
| EISCG2 | (CERN routine) calculates all the eigenvalues of a complex matrix. |
| F02AJF | (NAG routine) calculates all the eigenvalues of a complex matrix. Either one of the routines F02AJF or EISCG2 can be called for the same purpose. |
| FCN | Calculates the right-hand side of a system of first order differential equations. Called by the integration routine D208. |
| HPA | Calculates the HPA polynomials $P(x)$, $Q(x)$, $R(x)$, and $U(x)$ of order $m=2$ from Eq. (1.2). It references the routine SYSTEM. |
| INDEXB | Calculates the index β defined by Eq. (3.6). |
| INDEXS | Calculates the index s defined by Eq. (3.7). |
| MULLER | (CERN routine) computes the roots of a polynomial with real coefficients. |
| QUOTIENT | Calculates the quotient of the polynomial $P(x)$ by $(z - z_c)$. |
| SCAN | Scans the roots of the polynomial $P(x)$ and detects the most dominant singularity and the closest pair of roots for the case of confluent singularity. For the latter case, it calculates the center of the square and its side for the contour integration. |
| SYSTEM | Solves a $N \times N$ system of linear equations with real coefficients. It calls the routine COLMAX. |
| TAYLOR | Expands the polynomials $P(x)$, $Q(x)$, $R(x)$, $U(x)$ about the point z_c in powers of $\xi = z - z_c$. It calculates the coefficients $\{a_n\}$, $\{b_n\}$, and $\{c_n\}$ of the series solutions (3.19)–(3.20). |
| TESTS | Derives a series expansion for an assigned test function. |
| ZPOLR | (IMSL routine) computes the roots of a polynomial with real coefficients. |

4.5.1. Table of approximants

SUBROUTINE APPTAB (N1, NPADE, ICONSTRA, NSEQ)

APPTAB constructs a table of approximants for a specific sequence, indicated by the INPUT parameter NSEQ. Convergence properties for various sequences of approximants have been proved elsewhere [3]. The

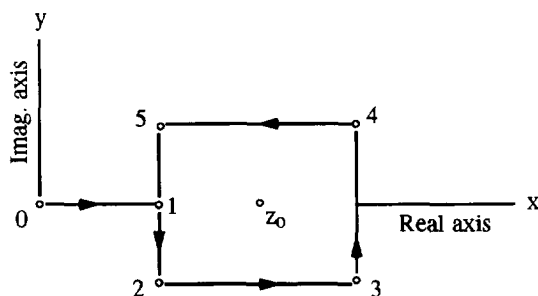


Fig. 1. A square contour of integration in the complex plane. z_0 is the center of the square and D its side. The sides of the square have been drawn parallel to the x -axis and the y -axis, respectively.

number of series terms available (INPUT) puts an upper bound for the highest order of approximants, since

$$\text{MDIM} + \text{LPJ} + \text{MPJ} + \text{LAJ} + \text{JPJ} = N1 \equiv N + 1.$$

If the degree of a polynomial is set equal to -1 , the polynomial is omitted altogether. Baker et al. [8] have studied invariance properties of the integral approximant. That has led to a specific sequence of approximants $[N/N, N+3, N+4]$, called “constrained” approximants, when a constraint is imposed on the polynomial coefficients,

$$q_{N+3} = 2p_{N+4}.$$

The constraint is activated from the parameter $\text{ICONSTRA} = 1$, or 0 (yes, or no).

4.5.2. Contour integration

SUBROUTINE CONTOUR ($y_0, Dy_0, z_0, D, W, DW, \text{eps}, z, \text{NLAPS}, \text{IER}$)

An integration contour is carefully drawn by the routine SCAN, on one hand to enclose one or more chosen singular points (Fig. 1) and on the other hand, not to intercept any other singular point. The latter will cause instability in the integration process. z_0 is the center and D the side of the square. The integration procedure is applied piecewise along a rectilinear piece from point z_{start} to point z_{end} in the complex plane, with given initial conditions $y(0) = y_0$ and $y'(0) = Dy_0$.

Local variables

$\text{NLAPS} = 2 \times \text{MDIM} + 1 = 5$ Number of laps for the contour integration.

$W(i); i=1,6$ Complex vector storing the values $y_n(z_1)$ of the monogenic analytic function calculated at the point $z = z_1$ (point 1 in Fig. 1).

$DW(i); i=1,6$ Complex vector storing the values of the derivatives $y'_n(z_1)$ at the point $z = z_1$.

Y_1, Y_2 The complex dependent variables y, y' .

z Complex independent variable of integration.

SUBROUTINE SCAN ($Z, \text{IR}, Zc_1, Zc_2, Iz_0, z_0, \text{SIDE}, \text{ZCFE}, \text{NZC}, \text{TYPE}, \text{IER}$)

The roots scanning procedure is obviously very sensitive to the degree of the accuracy sought on the results. It is possible for the approximation procedure to generate close pairs of spurious or accidental unphysical singularities. To protect the program from crashing or producing meaningless results, we force the routine SCAN to search for confluency or other type of singularities only among those roots lying close to the singular points we supplied as an input (from a previous run, or from guesses) to be searched for. This is done in the statement of the main program:

```

105 NZC = KI
DO 97 I = 1, NZC
97 READ(2) ZCFE(I)
GOTO 100

```

On return from SCAN, the complex vector $Z(\cdot)$ contains the following estimates:

Zc_1 most dominant singularity detected,

Zc_2 next dominant singularity, or the second member of the confluent pair.

On return, variable TYPE is assigned to the character value 'CONFLUENT' or 'NONCONFLU', depending on the type of singularities being detected. In the case of a confluent singularity, the center and the side of the square contour, (z_0 , SIDE), have been computed for the path integration to follow.

SUBROUTINE FCN (z, y, f, IER)

If we put $y_1 = y$ and $y_2 = y'$, the second order differential equation (3.1) is equivalent to the system

$$\begin{aligned}
 y_1' &= y_2, \\
 y_2' &= -\frac{Q(z)y_2 + R(z)y_1 + U(z)}{P(z)}.
 \end{aligned}$$

FCN computes the r.h.s. of this system and returns the values as elements of the array $f(2)$. If the computed values are extremely big, then the error message indicator IER is set to a nonzero value. This is the case when a singularity resides very close to the integration path.

5. The test run

The examples of this section are intended to illustrate typical behaviour of the method. We have chosen two test functions to apply the method. Both have dominant singularity at $x = z_1 = 1$. Function J has an additive singularity at the point $x = -\frac{5}{4}$, while function V has a confluent singularity at $x = z_1 = 1$ and an additive singular terms diverging at the point $x = \pm 3$. These test functions have been expanded to as many as 50 terms;

$$\begin{aligned}
 J: W(x) &= (1-x)^{-1.5} + (1 + \frac{4}{5}x)^{-1.25}, \\
 V: W(x) &= (1-x)^{-1.75} + (1-x)^{-1.25} + \sqrt{\frac{1 - \frac{1}{3}x}{1 + \frac{1}{3}x}}.
 \end{aligned}$$

In the disk of convergence of the nearest singularity $z = 1$, test function J has a local monodromic dimension $m = 1$ + analytic background (the global monodromic dimension is $m = 2$). Overall, there are two isolated singularities with the structure of Eq. (3.17) and the critical parameters

$$\begin{aligned}
 z_1 = 1: \quad \gamma &= -1.5, \quad \phi_1 = i, \quad \phi_0 = 1.8^{-1.25}, \\
 z_2 = -\frac{5}{4}: \quad \gamma &= -1.25, \quad \phi_1 = 0.8^{-1.25}, \quad \phi_0 = 2.25^{-1.5}.
 \end{aligned}$$

It can be easily shown that function J satisfies the equation

$$(1 - 0.12x - 0.816x^2 - 0.064x^3)w'' - (0.78 + 3.84x + 0.24x^2)w' - (2.58 + 0.12x)w = 0,$$

therefore, function J can be represented exactly by the approximant $[-1/1, 2, 3]$.

In the disk of the nearest singularity $z = 1$ test function V has a local monodromic dimension $m = 2$ + analytic background, i.e., it exceeds that of the approximant (the global monodromic dimension of the

Table 1

Estimates of the critical parameters for the test functions J and V presented in Section 5 (the numbers tabulated are the quantities $\varepsilon = -\log_{10} |(X - X_{\text{exact}})/X_{\text{exact}}|$)

| | | | | | | | | | |
|--------------------------|----------|-----|-------|------------|------------|------------|----------|------------|----------|
| Isolated singularities: | Function | n | z_1 | γ_1 | ϕ_1 | ϕ_0 | z_2 | γ_2 | |
| | J | 10 | 15.7 | 14.8 | 12.0 | 10.9 | 15.7 | 14.6 | |
| Confluent singularities: | Function | n | z_1 | z_2 | γ_1 | γ_2 | ϕ_1 | ϕ_2 | ϕ_0 |
| | V | 10 | 3.1 | 0.4 | 1.4 | – | – | – | – |
| | | 15 | 3.5 | 0.6 | 1.5 | – | – | – | – |
| | | 20 | 3.7 | 1.7 | 1.4 | 0.8 | 0.6 | 0.4 | 1.6 |
| | | 25 | 4.1 | 2.5 | 2.0 | 1.3 | 1.2 | 0.8 | 1.2 |
| | | 30 | 4.3 | 3.3 | 2.7 | 2.0 | 1.9 | 1.6 | 1.7 |
| | | 35 | 4.6 | 4.1 | 3.7 | 2.9 | 4.2 | 2.7 | 2.5 |
| | | 40 | 6.2 | 6.2 | 5.6 | 5.2 | 4.2 | 4.2 | 4.2 |

function is $m = 3$). Globally, there is a confluent singularity at $z = 1$ and two isolated singularities at $z = \pm 3$ with the parameters

$$z_1 = z_2 = 1 : \quad \gamma_1 = -1.75, \quad \gamma_2 = -1.25, \quad \phi_1 = e^{-1.75\pi i}, \quad \phi_2 = e^{-1.25\pi i}, \quad \phi_0 = \frac{1}{\sqrt{2}},$$

$$z_3 = -3 : \quad \gamma = -0.5, \quad \phi_1 = \sqrt{6}, \quad \phi_0 = 4^{-1.75} + 4^{-1.25}, \quad \text{etc.}$$

Estimates of the dominant singular points, the critical exponents and the amplitudes for the test functions J and V are tabulated in Table 1, as a function of the number of series terms used in the approximation. The registered numbers on the table are the quantities $\varepsilon = -\log_{10} |(X - X_{\text{exact}})/X_{\text{exact}}|$, i.e., the number ε roughly represents the number of significant figures in the estimation of the corresponding critical parameter. The rate of convergence of the estimates depends mainly on the type of singularity in investigation. In many cases, a proper variable transformation can eliminate additive singularities from the disk of convergence, and as result the convergence rate may be improved. At the end of the program tape we have included the run outputs for the test functions J and V .

6. Concluding remarks

We have presented a program implementing the Hermite–Padé approximation scheme based on monodromy and Riemann's theorem. We have reviewed the monodromy theory from the classical analysis of multivalued functions. Application of the method on test functions and on realistic series support the effectiveness of the method. The method provides a powerful approach for studying confluent singularities and revealing, in general, the character of multivalued functions. Extensive explanations on the algorithm are included for easier use of the code.

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TEST RUN OUTPUT

This is the output file 'HPA.OUT1' (selected results from the test run output using the test function J)

RUN OUTPUT FROM PROGRAM = IA.FOR

TOLERANCE= 0.1000E-14 (FOR THE INTEGRATING ROUTINES TOL= 0.1000E-13)

TEST 1

TEST FUNCTION J: $(1-X)^{-1.50} + (1+4/5 X)^{-1.25}$

TABL 2

HORIZONTAL SEQUENCES : [N/0,0,1->3] & [N/1,2,1->3] , ORDERS

*** 4. INTEGRAL APPROXIMANT [-1/ 1, 2, 3] 10-SERIES COEFFS CONSUMED IER(HPA)= 1

HPA POLYNOMIAL COEFFS: P(3),Q(2),R(1),U(-1)

(solution credibility in SYSTEM: -0.24619922484846290100D-01 * X(8) = 0.29543906981775724940D-02)

0.10000000000000000000000000D+01

-0.12000000000006849631973D+00

-0.81599999999998669431012D+00

-0.63999999999945199682938D-01

-0.779999999999412858553D+00

-0.3839999999999505084780D+01

-0.2399999999974401532210D+00

-0.25800000000000015143442D+01

-0.1199999999983824820748D+00

| ROOTS OF P(X): REAL PART | IMAG. PART | INDEX BETA: REAL PART | IMAG. PART |
|-----------------------------------|----------------------------|-----------------------------------|----------------------------|
| -0.12500000000107092112955343D+02 | 0.00000000000000000000D+00 | 0.200000000000078320683272182D+01 | 0.00000000000000000000D+00 |
| -0.12499999999999972244424384D+01 | 0.00000000000000000000D+00 | -0.12499999999999678035322859D+01 | 0.00000000000000000000D+00 |
| 0.999999999999819588758498D+00 | 0.00000000000000000000D+00 | -0.1499999999999744648704336D+01 | 0.00000000000000000000D+00 |

A NONCONFLU SINGULARITY DETECTED BY SCAN AT: ZC1= 0.100000000000E+01 0.000000000000E+00

Critical amplitudes for an isolated singularity at ZC= 1.000000000 0.000000000

AMPL1 = -0.806628049470958E-14 0.99999999999859E+00 AMPL0 = 0.479633345213556E+00 -0.931025460350620E-29

This is the output file 'HPA.OUT2' (selected results from the test run output using the test function V)

RUN OUTPUT FROM PROGRAM = IA.FOR

TOLERANCE= 0.1000E-14 (FOR THE INTEGRATING ROUTINES TOL= 0.1000E-13)

MONODROMIC DIMENSION = 2

TEST 1

TEST FUNCTION V.: $(1-X)^{-1.75} + (1-X)^{-1.25} + [(1-X/3)/(1+X/3)]^{**} 0.50$

X(1)= 3.00000000000000000000000000

X(2)= 2.666666666666666666668517038374375

X(3)= 3.8680555555555555558022717832500

X(4)= 4.51273148148148151026504137917

X(5)= 5.19505931712962965018931527084

X(6)= 5.80558569637345678327022824305

TABL 2

HORIZONTAL SEQUENCES : [N/0,0,1->3] & [N/1,2,1->3] , ORDERS

*** 24. INTEGRAL APPROXIMANT [24/ 1, 2, 3] 35-SERIES COEFFS CONSUMED IER(HPA)= 0

HPA POLYNOMIAL COEFFS: P(3),Q(2),R(1),U(24)

(solution credibility in SYSTEM: 0.95112943557426497462D-02 * X(33) = 0.10755570289963140245D-11)

0.10000000000000000000000000D+01

-0.16364460920462604587300D+01

0.27295740519196026035997D+00

0.36348868423844327146810D+00

-0.39744714307405204500867D+01

0.24975055440650189009233D+01

```

ROOTS OF P(X): REAL PART      IMAG. PART      INDEX BETA: REAL PART      IMAG. PART
-0.275098567481674161072646712D+01  0.113413027459846789245D-30  0.935251272619189749635282283D+00  0.116967830556335793918D-30
0.100007382795180206237173254D+01  0.426196180369178362910D-26  -0.651953523381325783514483874D+00  -0.296379476977613320903D-22
0.999974012957284275060487744D+00  -0.426207521671924347589D-26  -0.134611544414716532980236252D+01  0.296379475807958186841D-22

```

A CONFLUENT SINGULARITY PAIR DETECTED BY SCAN: ZC1= 0.9999740130E+00-0.4262075217E-26 ZC2= 0.1000073828E+01 0.4261961804E-26
 APPROXIMATE VALUES FOR THE CRIT. INDICES: GAMMA1=(-0.17496327D+01,-0.58482757D-31) GAMMA2=(-0.12484362D+01,-0.58482757D-31)

```

INTEGRATION ALONG A SQUARE CONTOUR: CENTERED AT Z0= 0.100002392045E+01 0.000000000000E+00 SIDE= 0.1000E+00
Z= 0.95002272443E+00 0.000000000000E+00 W1= 0.23233814904E+03 0.000000000000E+00 W1'= 0.76866590166E+04 0.000000000000E+00 NFC= 50615
Z= 0.95002272443E+00 0.000000000000E+00 W2= 0.69300376178E+00 0.14719703854E+03 W2'= -0.52903355791E+01 0.55764595250E+04 NFC= 128165
Z= 0.95002272443E+00 0.000000000000E+00 W3= -0.23089199343E+03 -0.17069890339E+01 W3'= -0.76869182569E+04 -0.51469754122E+02 NFC= 128165
Z= 0.95002272443E+00 0.000000000000E+00 W4= 0.79311347300E+00 -0.14720922507E+03 W4'= 0.14806993826E+02 -0.55767233676E+04 NFC= 128165
Z= 0.95002272443E+00 0.000000000000E+00 W5= 0.23229747899E+03 0.34136400014E+01 W5'= 0.76855607142E+04 0.10293086780E+03 NFC= 128165
Z= 0.95002272443E+00 0.000000000000E+00 W6= 0.59229354397E+00 0.14723359195E+03 W6'= -0.25402298311E+02 0.55772508992E+04 NFC= 128165

```

```

MONODROMY MATRIX
0.000000000000E+00 0.000000000000E+00 0.100000000000E+01 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00
0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.000000000000E+00 0.100000000000E+01 0.000000000000E+00
0.999992395634E+00 0.121327371657E-01 -0.100742110192E+01 -0.121782044920E-01 0.100749470629E+01 0.454673219657E-04

```

```

IER=0 EIGENVALUES= 0.981379076285E-02 -0.999951843596E+00
0.999999999999E+00 -0.21416835191E-11
-0.231908447389E-02 0.999997310920E+00

```

```

EIGENVALUE = 0.981379114091E-02 -0.999951839447E+00
GAMMA = -2.248438061617
-1.248438061617
-0.248438061617
0.751561938383
1.751561938383
2.751561938383

```

```

EIGENVALUE = -0.231908448040E-02 0.999997317791E+00
GAMMA = -1.749630905912
-0.749630905912
0.250369094088
1.250369094088
2.250369094088
3.250369094088

```

CRITICAL AMPLITUDES FOR A CONFLUENT SINGULARITY AT ZC = 0.99997401295728427506049E+00-0.42620752167192434758853E-26
 (select the correct values from the correct Riemann sheet, guided from the approximate values of the critical indices)

```

GAMMA1=-2.248438061617 AMPL1= 0.978075521757E-05 -0.968578178299E-05
GAMMA1=-1.248438061617 AMPL1=-0.711836917655E+00 0.704885074245E+00
GAMMA1=-0.248438061617 AMPL1= 0.284973235219E+02 -0.282190166772E+02
GAMMA1= 0.751561938383 AMPL1=-0.855714168273E+03 0.847357201964E+03
GAMMA1= 1.751561938383 AMPL1= 0.228407734746E+05 -0.226177088035E+05
GAMMA1= 2.751561938383 AMPL1=-0.571568320407E+06 0.565986341779E+06
GAMMA2=-1.749630905912 AMPL2= 0.706334982543E+00 0.707974941395E+00
GAMMA2=-0.749630905912 AMPL2=-0.282908898800E+02 -0.283565752726E+02
GAMMA2= 0.250369094088 AMPL2= 0.849653838638E+03 0.851626552980E+03
GAMMA2= 1.250369094088 AMPL2=-0.226808584760E+05 -0.227335185735E+05
GAMMA2= 2.250369094088 AMPL2= 0.567594344717E+06 0.568912177255E+06
GAMMA2= 3.250369094088 AMPL2=-0.136358676991E+08 -0.136675272640E+08
AMPL0= 0.704663956446E+00 0.394349671316E-07

```